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Pure entangled states probed by multipartite Bell experiments

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The spectral decomposition of all $(n, 2, 2)$ Bell operators (2^{2^n} in number, $n \geq 2$), as introduced by Werner and Wolf [7], is done. Its implications on the characterization of Bell operators as probes of entanglement are considered in detail.

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I. INTRODUCTION

Bell experiments are designed to test correlations that are supported by local realistic models [3]. A general experimental setup consists of n observers, each of them is given a particle and, independently, decide what of m observables, which are v-valued each, to measure. All such setups constitute the (n, m, v) Bell experiment. One setup in the (n, m, v) class may be tuned up in one of m^n forms and in each of its forms it detects one of v^n data instances. Bell inequalities are constraints that local realistic models impose to the experimental correlation functions.

The set of CHSH inequalities[2] is complete for the $(2, 2, 2)$ class. Mermin's example [4] generalizes CHSH inequalities to the $(n, 2, 2)$ class, where a complete set of inequalities grows as 2^{2^n} [7, 8] in cardinality. A complete theory of $(n, 2, 2)$ Bell experiments was developed by Werner and Wolf in [7].

In the quantal theory the measurement in a Bell experiment corresponds to a hermitian operator B. For a state ψ, the equivalent to Bell's inequality is $|\mathrm{tr}(\psi B)| \leq 1$. Every separable state satisfies the inequality. Stronger quantal correlations may violate it. When this happens for some state ψ we say experiment B probes entanglement.

We consider the infinite sequence of Bell operators for $(n, 2, 2)$ experiments, the largest class of experimental setups for which a complete theory is available [7]. We assume the observables $A_k(0)$ and $A_k(1)$ per particle $k \in \{1, \ldots, n\}$ with $A_k(s_k)^2 = \mathbb{1}$, $s_k = 0, 1$. In the theory [7], for each n, every Bell operator, B_f, has index f that takes value in the set $\{-1, 1\}^{2^n}$, of cardinality 2^{2^n}. The set of B_f operators is complete.

How a measurement B_f must be in order to detect pure entangled states? Answer to this question is important since the number of Bell inequalities grows exceedingly fast with n. For the $(2, 2, 2)$ class, Gisin's theorem [5] says that every pure nonproduct state of two particles violates a CHSH [2] inequality. However, the converse to Gisin's theorem is not true. Actually, an experiment B_f does not detect every pure entangled state. Several examples considered by Braunstein *et al.* [1] show that for detectability of pure entangled states in a $(2, 2, v)$ setup it is necessary that an eigenspace $\mathcal{H}_\lambda$ of B^2 with a degenerate eigenvalue $\lambda^2 > 1$ exists. I.e, $\dim(\mathcal{H}_\lambda) > 1$ for some $\lambda > 1$.

A general technical lemma (Lemma III.1) lead us to the characterization of a $(n, 2, 2)$ Bell experiment by the following equivalent assertions.

(1.a) B_f is a probe of entangled states.
(1.b) B_f has spectral radius greater than one.
(1.c) There exists an eigenspace $\mathcal{H}_\lambda$ of B_f^2 with $\dim(\mathcal{H}_\lambda) > 1$ for some $\lambda > 1$.

We are expressing characteristics of B_f in terms of those ones of B_f^2 because in Section II we show that B_f^2 has a simple spectral decomposition and the set of eigenstates constitutes a "natural" product basis for the state space, $\mathcal{H}$. Main results on B_f^2 are proved in Appendix A. In particular, formulae are given to compute the spectral radius, Λ_f, of B_f in terms of the geometric parameters of the experimental setup, for each f. The spectral radius Λ_f is the largest factor of violation that is detectable by experiment B_f. The maximal violation factor that is allowed in principle for $(n, 2, 2)$ Bell experiments was determined by Werner and Wolf in [7] to be $\Lambda_n \equiv 2^{(n-1)/2}$. I.e., $\Lambda_f \leq \Lambda_n$ for every f. The equality holds, e.g., for Mermin's example.

Once we know that B_f detects entanglement, by a violation factor of at most Λ_f, we want a finer characterization of it. What entangled states are detectable by B_f? What f and what geometry make experiment B_f to admit the maximal violation factor Λ_n that is allowed *in principle*?

The spectrum λ_f^2 of B_f^2 satisfies the sum rule

$$\sum_w \lambda_f^2(w) = \dim(\mathcal{H}) = 2^n \ , \tag{1}$$

where w is an index for the eigenstates of B_f^2. The total spectrum (1) is independent of f and of geometric parameters. Thus, the difference between experiments is how the total spectrum is distributed among states. In extreme situations are an experiment with spectrum equally distributed among all states and an experiment with spectrum concentrated in just two states. In the first case the sum rule (1) implies that $\lambda_f(w) = 1$ and the experiment does not detect entanglement. In the second case sum rule (1) implies that the maximal violation factor Λ_n is admitted by the experiment. Thus,

we say that f is optimal if B_f has a geometry where $\Lambda_f = \Lambda_n$. An experiment B_f is "optimal" in the sense that it "concentrates" the maximal factor of violation Λ_n in as few entangled states as possible. Such an experiment is the sharpest test for entanglement. The following equivalent assertions provide a characterization of optimal $(n, 2, 2)$ Bell experiments.

(2.a) B_f has spectral radius Λ_n
(2.b) f is optimal and $\|(i/2)[A_k(0), A_k(1)]\| = 1$ for each particle k.
(2.c) The Bell inequality is violated by two and only two eigenstates of B_f.

We find that, *for each n, there are four optimal $(n, 2, 2)$ Bell experiments of which only two are independent.* A very small number as compared with 2^{2^n}, even for small n. And only two of their eigenstates violate Bell's inequality. I.e., (2.c) above.

A formula to compute the optimal values of f for each n is given. Optimal probes B_f are computed easily. We provide examples for $n = 2$, 3 and 4 in Appendix B. For $n = 2$ they are the CHSH operators [2] and for $n = 3$ the Bell polynomials were derived in [7].

The entangled character of the states detected by an optimal experiment depends on the geometry. Statement (2.b) has room for 2^n geometries. *For any f, all eigenstates of B_f are generalized GHZ states*: superposition of two states with antipodal configurations. For optimal f the sum rule (1) is saturated by just a pair of antipodal configurations. Every geometry determines a pair and there two geometries per pair. For example, in a CHSH setup there are four geometries that admit the maximal violation factor: two geometries "put" the violation factor on two EPR states and two other geometries put it on two GHZ states.

II. $(n, 2, 2)$ BELL OPERATORS

We consider the infinite sequence of Bell operators introduced by Werner and Wolf for which the theory is developed in [7] to be as explicite and complete as in the CHSH case. [2] To make the article self-contained, the next paragraph summarizes the main line of thought in [7].

Each $(n, 2, 2)$ Bell experiment admits a set $\mathcal{S} := \{0, 1\}^n$ of experimental setups. It is convenient to consider $\mathcal{S} \equiv \mathbb{Z}_2^n$. For every setup $s \in \mathcal{S}$ there is the correlation function $\xi(s) = \langle \prod_{k=1}^n A_k(s_k) \rangle$ which is considered to be the s-coordinate of vector ξ. The local-realistic hypothesis bounds vector ξ to lay in the convex hull Ω of the finite collection of vectors $\{\pm\epsilon_r : \ r \in \{0, 1\}^n\}$, with coordinates $\epsilon_r(s) = (-1)^{\langle r,s \rangle}$. The opposite is also true. This assertion is equivalent to say that $\langle \beta, \xi \rangle \leq 1$ for each vector $\beta \in \Omega^\circ$, the polar set of Ω. Being Ω° a polytope it is enough to ask that $\langle \hat{f}, \xi \rangle \leq 1$ for each maximal vector $\hat{f}$ of Ω°. Maximal vectors are found to be given by the Fourier transform on the group $\mathcal{S}$

$$\hat{f}(s) = 2^{-n} \sum_{r \in \mathcal{S}} (-1)^{\langle r,s \rangle} f(r) \ , \tag{2}$$

for each $f : \mathcal{S} \to \{-1, 1\}$.

In the quantal description the quantities $\langle \hat{f}, \xi \rangle = \sum_{s \in \mathcal{S}} \hat{f}(s) \langle \prod_{k=1}^n A_k(s_k) \rangle$ are replaced by the expectation value of the operators

$$B_f = \sum_{s \in \mathcal{S}} \hat{f}(s) \bigotimes_{k=1}^{n} A_k(s_k) \ , \tag{3}$$

one for each $f \in \{-1, 1\}^{2^n}$. The freedom we have to choose observables makes B_f to depend on geometric parameters. Thus, every vector f represents, not one, but a class of Bell operators.

In Appendix A we show that the operator B_f^2 is given by the formula

$$B_f^2 = \mathbb{1} + \sum_{\substack{p \subset \{1,\ldots,n\} \\ \#p \text{ is even}}} C_p(f) \bigotimes_{k \in p} \frac{i}{2} [A_k(0),\, A_k(1)] \tag{4}$$

where the sum is over all non-empty subsets of points $p \subset \{1, \ldots, n\}$ of even cardinality. Coefficients $C_p(f)$ depend on geometric parameters and they are $2^{n-1} - 1$ in number. Everyone is bounded to lay in the interval $[-1, 1]$,

$$|C_p(f)| \leq 1 \ . \tag{5}$$

Formulae to calculate $C_p(f)$ are given in Appendix A. Equality in (5) holds for a vector f in Mermin's example.

The spectral decomposition of Bell operator B_f in Section III follows from the simple spectral properties of operator B_f^2 in (4). For the moment, remark that each operator $(i/2)[A_k(0), A_k(1)]$ in (4) is hermitian and laying in the ball $\|A\| \leq 1$. Thus, it can be represented in the form

$$\frac{i}{2} [A_k(0),\, A_k(1)] = \sin \theta_k Z_k, \qquad \theta_k \in [-\pi/2,\, \pi/2] \ , \tag{6}$$

where each hermitian operator Z_k is traceless and maximal, $\|Z_k\| = 1$. The obvious choice is to take $Z_k = \sigma_3$, the same at each site k. It amounts to take $A_k(s_k) = \langle n_k(s_k), \sigma \rangle$ with unitary vector $n_k(s_k) = (\cos \varphi_k(s_k), \sin \varphi_k(s_k),\ 0)$ laying on the x-y–plane of a local coordinate system such that $n_k(1) \times n_k(0) = (0,\ 0,\ \sin \theta_k)$.

The orthonormal set $\{\, |w_k\rangle \ : \ w_k = -1, 1\}$ of eigenvectors of σ_3 is adopted as the basis of the state space $\mathcal{H}_k = \mathbb{C}^2$. The set of configurations $\mathcal{C}$ for the product basis of $\mathcal{H} = \mathbb{C}^{2 \otimes n}$ is $\mathcal{C} = \{-1, 1\}^n$. For each configuration $w = w_1 w_2 \cdots w_n \in \mathcal{C}$ there is the product vector

$$|w\rangle \ = \ |w_1\rangle \otimes |w_2\rangle \cdots \otimes |w_n\rangle \tag{7}$$

which is an element of the product basis of $\mathcal{H}$. Thus, each product vector (7) is an eigenvector of B_f^2 with eigenvalue

$$\lambda_f^2(w) = 1 + \sum_{\substack{p\subset\{1,\dots,n\} \\ \#p \text{ is even}}} C_p(f) \prod_{k\in p} w_k \sin\theta_k \quad \geq \quad 0 \ . \quad (8)$$

The spectral radius of B_f is $\Lambda_f := \max_w\{\lambda_f(w)\}$. It is attained by a configuration $W \in \mathcal{C}$ such that $C_p(f)\prod_{k\in p} W_k \sin\theta_k \geq 0$. I.e., $\Lambda_f = \lambda_f(W)$. The spectral radius may be computed with the formula

$$\Lambda_f = 1 + \sum_{\substack{p\subset\{1,\dots,n\} \\ \#p \text{ is even}}} |C_p(f)| \prod_{k\in p} |\sin\theta_k| \qquad (9)$$

and results on $C_p(f)$ in Appendix A.

The following symmetries of B_f^2 and its eigenvalues are apparent from (4) and (8).

(3.a) B_f^2 is invariant under the exchange of observables $A_k(0) \leftrightarrow A_k(1)$ at all points k. I.e., $\sin\theta_k \leftrightarrow -\sin\theta_k$ and there are at least two geometries that yield identical results.

(3.b) $\lambda_f(w) = \lambda_f(\tilde{w})$, where the configuration $\tilde{w} \in \mathcal{C}$ has coordinates $\tilde{w}_k = -w_k$. I.e., the eigenvalues of B_f^2 are at least doubly degenerate.

Due to the form (4) of B_f^2, the eigenvalues (8) satisfy sum rule (1). The value for the sum (1) is independent of any geometric parameter and of f.

Results (8) and (1) allow us to think of the spectral function λ_f^2 as a weight function on the set of configurations $\mathcal{C}$ with full weight $\#\mathcal{C} = 2^n$. The same amount of total weight is available to every experiment B_f, independent of f and of the choice of observables. The difference between experiments consists in the way they distribute the weight in the configuration set $\mathcal{C}$. An experiment that equally distributes the weight among all configurations does not probe entanglement since $\lambda_f^2(w) = 1$ for each $w \in \mathcal{C}$. This happens when $[A_k(0), A_k(1)] = 0$ at every point k.

Experiment B_f is a good probe of entanglement if the total weight $\#\mathcal{C}$ is supported in as few configurations as possible. In Section IV we will see that the "best" situation is when λ_f^2 concentrates all of the weight that is available, $\#\mathcal{C}$, on just two configurations.

III. ALL BELL EIGENSTATES ARE GHZ

The spectral decomposition of B_f^2 is simple enough as to base on it the corresponding decomposition of B_f. To proceed, remark that B_f^2 is a positive operator and it has a unique positive square root, denoted by $|B_f|$. Operator $|B_f|$ has the same set $\{\,|w\rangle\,\}$ of eigenvectors as B_f^2, with eigenvalues $\lambda_f(w) \geq 0$. Experiment B_f is decomposed into the product $B_f = S_f\,|B_f|$ where, in general, the operator S_f is an isometry. For the particular form of operator B_f in (3) a direct calculation shows that $B_f\,|w\rangle = \beta_f(w)\,|\tilde{w}\rangle$, with $|\beta_f(w)| = \lambda_f(w)$. Thus, up to a phase factor, S_f is the permutation,

$$S_f\,|w\rangle \,=\, |\overline{w}\rangle := e^{i\varphi_f(w)}\,|\tilde{w}\rangle \ , \qquad (10)$$

where the phase factor, whenever $\lambda_f(w) \neq 0$, can be written as

$$e^{i\varphi_f(w)} = \frac{\beta_f(w)}{\lambda_f(w)} \ . \qquad (11)$$

Furthermore, $S_f^2 = \mathbb{1}$. The properties of S_f are used in the following construction.

Let $\mathcal{H}_\lambda \subset \mathcal{H}$ be an eigenspace of B_f^2 corresponding to the eigenvalue λ^2. Consider product state $|w\rangle \in \mathcal{H}_\lambda$. By (10), the vectors

$$B_f\,|w\rangle \,=\lambda\,|\overline{w}\rangle \quad \text{and} \quad B_f\,|\overline{w}\rangle \,=\lambda\,|w\rangle$$

are orthonormal, in $\mathcal{H}_\lambda$ too. It is of course necessary that $\dim(\mathcal{H}_\lambda) > 1$. That it is so, follows from the properties of S_f. Then, the 2-d subspace span$\{\,|w\rangle\,,\,|\tilde{w}\rangle\,\} \subset \mathcal{H}_\lambda$ is S_f-invariant and every eigenvector of all Bell operators B_f is an entangled state of the form

$$|w;\pm\rangle \,=\, \frac{1}{\sqrt{2}}\,(\,|w\rangle \,\pm\, |\overline{w}\rangle\,) \qquad (12)$$

with eigenvalues $\pm\lambda = \pm\lambda_f(w)$. Any $(n,2,2)$ Bell experiment probes entanglement of states with antipodal configurations, w and $\tilde{w}$. Such pure states we call GHZ.

Remark that two GHZ states $|w;\pm\rangle$ and $|\tilde{w};\pm\rangle$ differ by just a phase factor. Thus, to deal with the eigenvectors of B_f we consider configurations in the quotient set $\mathcal{C}/{\sim}$, where antipodal configurations w and $\tilde{w}$ are equivalent.

That $\dim(\mathcal{H}_\lambda) > 1$ is a necessary and sufficient condition for the existance of pure entangled states that violate Bell inequality by the factor $\lambda > 1$ is proved in general in the following.

Lemma III.1 *Let $\mathcal{H}_\lambda$ be an eigenspace of B^2 of eigenvalue λ^2. Assume $\lambda > 1$. Then* (I) *there exists $|\,\rangle \in \mathcal{H}_\lambda$ such that*

$$|\,\langle\,|\,B\,|\,\rangle\,|\,>\,1 \qquad (13)$$

if and only if (II) $\dim(\mathcal{H}_\lambda) \geq 2$.

Proof. (II $\Rightarrow$ I). We are assuming that $\lambda^2 > 1$ is a degenerate eigenvalue of B^2. The eigenspace $\mathcal{H}_\lambda$ of B^2 is B-invariant. The restriction $B|_{\mathcal{H}_\lambda}$ is hermitian and thus it has eigenvectors $|\lambda\rangle \in \mathcal{H}_\lambda$ with eigenvalues λ such that $|\lambda| > 1$ Then, statement (I) follows. Remark that $|\lambda\rangle$ is not separable by necessity. Such eigenvectors were actually constructed in (12) for the particular form of the $(n,2,2)$ B_f operators.

Sufficiency is proved by contradiction ($\neg$II $\Rightarrow$ $\neg$I). We are assuming $\lambda > 1$ and by hypothesis ($\neg$II) the eigenspace $\mathcal{H}_\lambda$ of B^2 has $\dim(\mathcal{H}_\lambda) = 1$ (the case of zero dimension is trivial) and is spanned by the eigenvector

$|\lambda\rangle$. Since $\mathcal{H}_\lambda$ is B-invariant then $|\lambda\rangle$ is an eigenvector of B too. The contradiction stems from the fact that the unique state $|\lambda\rangle \in \mathcal{H}_\lambda$ is a product vector (7) for some configuration $w \in \mathcal{C}$ and then inequality (13) is violated by the only (separable) state $|w\rangle \in \mathcal{H}_\lambda$. □

In Section II we proved that each eigenvalue of B_f^2 is at least doubly degenerate. Thus Lemma III.1 applies and a corollary is the following characterization of $(n,2,2)$ Bell experiments as probes of entanglement: *B_f detects pure entangled states iff B_f^2 has a spectral radius that is greater than one.*

Eigenvectors of B_f come in entangled pairs of the GHZ form (12), two such states for each $w \in \mathcal{C}/\!\sim$. In the GHZ basis *all* $(n,2,2)$ Bell operators have the diagonal form $B_f = \mathrm{diag}(B_f(+), B_f(-))$ with diagonals

$$B_f(\pm) = \pm \sum_{w\in\mathcal{C}/\sim} \lambda_f(w)\, |w;\pm\rangle\langle w;\pm| \ .$$

Every entangled state that is detectable by experiment B_f is supported on the subspace $\mathcal{H}_> := \bigoplus_{\lambda>1} \mathcal{H}_\lambda$. The factors of violation associated with the entangled state (12) is $\lambda_f(w)$. The definition of state $|\overline{w}\rangle$ includes the phase factor (11) that we did not calculate.

IV. OPTIMAL PROBES

The upper bound $\Lambda_n = 2^{(n-1)/2}$ for the maximal possible violation factor of any $(n,2,2)$ Bell inequality was determined by Werner and Wolf in [7]. Here, directly from (4) and (5), we see that

$$\begin{aligned}\Lambda_f \ &\leq\ \max_f \|B_f^2\|^{1/2} \leq \left(1 + \sum_{m=1}^{\lfloor n/2 \rfloor} \binom{n}{2m}\right)^{1/2} \\ &\leq\ 2^{(n-1)/2} \ . \end{aligned} \qquad (14)$$

The bound is attained by an experiment B_f with a configuration w and geometry such that

$$|w_k \sin\theta_k| = \|\frac{i}{2}[A_k(0), A_k(1)]\| = 1.$$

and a vector $f \in \{-1,1\}^{2^n}$ such that $\overline{C}_p(f) = 1$, where $\overline{C}_p(f)$ is the value of $C_p(f)$ when geometric parameters are $\cos\theta_k = 0$. A formula for $\overline{C}_p(f)$ is given in Appendix B, formula (B1).

Under such conditions, formula (8) gives $\lambda_f^2(w) = 2^{n-1}$ as the largest eigenvalue possible for the given B_f^2. Thus, *the $(n,2,2)$ Bell experiment B_f has maximal spectral radius $\Lambda_n = 2^{(n-1)/2}$ if and only if $\overline{C}_p(f) = 1$ and* $\|(i/2)[A_k(0), A_k(1)]\| = 1$.

Let us assume experiment B_f admits the maximal violation factor $\Lambda_n = 2^{(n-1)/2}$. Then, according to Lemma III.1, the corresponding Bell inequality is violated iff there exists at least two eigenstates $|w\rangle$ and $|\overline{w}\rangle$ of B_f^2 with eigenvalue $\lambda_f^2(w) = \lambda_f^2(\overline{w}) = 2^{n-1}$. But two such states saturate the sum rule (1) and there can not be any other eigenstate involved in the violation of Bell inequality (just one state is not enough because eigenstates of B^2 are separable). Thus, in experiments of maximal violation, the spectrum λ_f^2 equally distributes weight $\#\mathcal{C}$ in just two configurations (no less, no more). This proves that *B_f has spectral radius Λ_n if two and only two of its eigenstates violate the corresponding Bell inequality.*

Experiments of maximal violation are optimal probes of entanglement in that they are tunable as to detect any given configuration w by choosing the sign of $\sin\theta_k = \pm 1$ such that $w_k \sin\theta_k = 1$. In an optimal Bell experiment λ_f^2 concentrates all weight that is available in just two GHZ states of our choice: $|w;+\rangle$ and $|w;-\rangle$.

Looking at formula (B1) for $\overline{C}_p(f)$ we immediately see that a vector f that satisfies the conditions

$$f(s)f(s+p) = (-1)^{\langle p,s\rangle + \#p/2}, \qquad (15)$$

is an optimal one with $\overline{C}_p(f) = 1$. In (15), $s \in \mathcal{S}$ and the subset $p \subset \{1,\ldots,n\}$, of even cardinality, is represented by the vector $p \in \mathcal{S}$ with coordinate $p_k = 1$ iff $k \in p$. Remark that for any two subsets p and p' of even cardinality, the symmetric difference $p + p'$ (coordinate-wise mod 2 addition) is also of even cardinality. The collection $\mathcal{P}_n := \{p : \ \#p = \text{even}\}$ (when $0\cdots 0$ is included) is a subgroup of $\mathcal{S}$ of order 2^{n-1}. So the set of independent conditions (15) lay on the orbits of two setups. E.g., $s = 0\cdots 00$ and $s = 0\cdots 01$. The sign of the coordinates of f may be assigned in just two ways to each orbit. Thus, *for each n, there are four optimal $(n,2,2)$ Bell experiments of which only two are independent.*

Optimal probes of entanglement for any number n of particles are computed easily by using formula (15). Probes for $n = 2$ (the CHSH operators[2]), $n = 3$ (derived in [7]) and $n = 4$ are obtained in Appendix B.

APPENDIX A: THE OPERATOR B_f^2

Results (4) and (5) about B_f^2 are obtained in the following.

From definition (3) we have that

$$\begin{aligned} B_f^2 \ &=\ \sum_{s,s'\in\mathcal{S}} \hat{f}(s)\hat{f}(s') \bigotimes_{k=1}^{n} A_k(s_k)A_k(s'_k) \\ &=\ \sum_{s,s'\in\mathcal{S}} \hat{f}(s)\hat{f}(s')\mathcal{O}(s,s') \end{aligned} \qquad (A1)$$

where

$$\mathcal{O}(s,s') = \mathrm{Sym}_{s,s'} \bigotimes_{k=1}^{n} \left(\Phi_k(s_k,s'_k) + i\Gamma_k(s_k,s'_k)\right) \qquad (A2)$$

is the symmetric component of the tensor-product operator in (A1). I.e., $\mathcal{O}(s,s') = \mathcal{O}(s',s)$. In (A2) we have

made use of the following definitions

$$\begin{aligned}\Phi_k(s_k,s'_k) &:= \frac{1}{2}\{A_k(s_k),A_k(s'_k)\}\\ &= \mathbb{1}\frac{1+(-1)^{s_k+s'_k}}{2} \qquad \text{(A3)}\\ &\quad +\frac{1}{2}\{A_k(0),A_k(1)\}\frac{1-(-1)^{s_k+s'_k}}{2}\end{aligned}$$

and

$$\begin{aligned}\Gamma_k(s_k,s'_k) &:= \frac{-i}{2}[A_k(s_k),A_k(s'_k)] \qquad \text{(A4)}\\ &= \frac{(-1)^{s_k}-(-1)^{s'_k}}{2}\ \frac{i}{2}[A_k(1),A_k(0)]\ ,\end{aligned}$$

The hermitian operators $\Phi_k(s_k,s'_k)$ and $\Gamma_k(s_k,s'_k)$ are symmetric and anti-symmetric, respectively, under the exchange $s_k \leftrightarrow s'_k$. Furthermore, under the assumption that $A_k(s_k)^2=\mathbb{1}$, we have that

$$[\Phi_k(s_k,s'_k),\Gamma_k(s_k,s'_k)]=0\ .$$

These properties allow us to write the symmetric operator (A2) in the following form,

$$\mathcal{O}(s,s') = \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}} \bigotimes_{k\in p^c}\Phi_k(s_k,s'_k)\bigotimes_{k\in p}\Gamma_k(s_k,s'_k)\ , \qquad \text{(A5)}$$

where the sum is over subsets $p\subset\{0,\ldots,n\}$ of even cardinality, including $p=\emptyset$.

Substituting (A5) in (A1) we obtain

$$\begin{aligned}B_f^2 &= \mathbb{1} + \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}}(-1)^{\#p/2}\sum_{s,s'\in\mathcal{S}}\hat{f}(s)\hat{f}(s')\\ &\qquad \bigotimes_{k\in p}\Gamma_k(s_k,s'_k)\bigotimes_{\ell\in p^c}\Phi_\ell(s_\ell,s'_\ell) \qquad \text{(A6)}\end{aligned}$$

where the term $\mathbb{1}$ is the contribution from $p=\emptyset$ and the sum now runs over non-empty subsets. Considering in (A6) that $(1/2)\{A_k(0),A_k(1)\}=a_k\mathbb{1}$ with $a_k=\cos\theta_k$, we get formula (4) for B_f^2 with coefficients, at the moment, given by

$$C_p(f) = (-1)^{\#p/2}2^{-n}F_f(p) \qquad \text{(A7)}$$

where

$$F_f(p) := \sum_{s,s'\in\mathcal{S}}\hat{f}(s)\hat{f}(s')\prod_{k\in p}\gamma(s_k,s'_k)\prod_{\ell\in p^c}\varphi_k(s_k,s'_k)\ , \qquad \text{(A8)}$$

$$\gamma(s_k,s'_k) = (-1)^{s_k}-(-1)^{s'_k} \qquad \text{(A9)}$$

and

$$\varphi_k(s_k,s'_k) = 1+(-1)^{s_k+s'_k}+a_k(1-(-1)^{s_k+s'_k})\ . \qquad \text{(A10)}$$

The products in (A8), using (A9) and (A10), expand to

$$\prod_{k\in p}\gamma(s_k,s'_k) = \sum_{r\subset p}(-1)^{\#r}(-1)^{\sum_{k\in r}s'_k+\sum_{k\in r^c}s_k}\ , \qquad \text{(A11)}$$

where $r\cup r^c=p$, and to

$$\begin{aligned}\prod_{k\in p^c}\varphi_k(s_k,s'_k) &= \sum_{q\subset p^c}(-1)^{\sum_{k\in q^c}(s_k+s'_k)}\prod_{k\in q}(1+a_k)\\ &\qquad \prod_{k\in q^c}(1-a_k)\ , \qquad \text{(A12)}\end{aligned}$$

where $q\cup q^c=p^c$. The result for $F_f(p)$ in (A8) with the products expanded is

$$F_f(p) = \sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_k)\sum_{r\subset p}(-1)^{\#r}G(q,r) \qquad \text{(A13)}$$

where

$$G(q,r) = \sum_{s,s'\in\mathcal{S}}\hat{f}(s)\hat{f}(s')(-1)^{\sum_{k\in(q\cup r^c)}s_k+\sum_{k\in(q\cup r)}s'_k}\ . \qquad \text{(A14)}$$

For the following, it is convenient to denote subsets $q\subset\{1,\ldots,n\}$ by vectors $q\in\mathcal{S}$ such that $k\in q$ iff $q_k=1$ (we are abusing notation but no confusion will arise). With this identification, $G(q,r)$ in (A14) is seen to be the product of two inverse Fourier transforms,

$$G(q,r) = f(q+\overline{r})f(q+r)\ , \qquad \text{(A15)}$$

where $q\cup r\leftrightarrow q+r$ (because $qr=0$) and $r+\overline{r}=p$. Formula (A15) shows us that

$$|G(q,r)| = 1\ . \qquad \text{(A16)}$$

We have everything to prove inequality (5). From (A7) and (A13) we have that

$$|C_p(f)| \le 2^{-\#p^c}\sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_k)$$

where we have made use of (A16) and the fact that $|a_k|\le 1$. One proves by induction in $\#p^c$ that

$$\sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_k) = 2^{\#p^c} \qquad \text{(A17)}$$

and the inequality (5) follows. Our final answer for $C_p(f)$ consists of formulae (A7), (A13) and (A15).

APPENDIX B: EXAMPLES

The geometric parameters in optimal probes are settled down to $a_k=0$. I.e., $\sin\theta_k=\pm1$. Using the results obtained in Appendix A, the value $\overline{C}_p(f)$ of the coefficient (A7) for $a_k=0$ is

$$\overline{C}_p(f) = (-1)^{\#p/2}2^{-n}\sum_{s\in\mathcal{S}}(-1)^{\langle p,s\rangle}f(s)f(s+p)\ , \qquad \text{(B1)}$$

for each non-empty subset $p \subset \{1, \dots, n\}$ of even cardinality. A vector f that satisfies conditions (15) makes $\overline{C}_p(f) = 1$ and corresponds to an optimal experiment B_f. Optimal vectors for $n = 2$, 3 and 4 are computed in the following.

For $n = 2$ we have that $\mathcal{P}_2 = \{11\}$, that corresponds to the only subset $p = \{1, 2\}$. The orbits of setups 00 and 01 for conditions(15) are

$$f(00) = -f(11) \quad \text{and} \quad f(01) = (10) \; . \tag{B2}$$

For instance the vector $f = (1,\ 1,\ 1,\ -1)$, with Fourier transform $\hat{f} = (1/2,\ 1/2,\ 1/2,\ -1/2)$, is optimal and corresponds to one of the CHSH operators.

For $n = 3$ we have the collection $\mathcal{P}_3 = \{011, 101, 110\}$ that produce the two orbits

$$\begin{aligned} f(000) = -f(011) = -f(101) = -f(110) \; , \\ f(001) = f(010) = f(100) = -f(111) \; . \end{aligned} \tag{B3}$$

Two independent choices of sign in (B3) give the vectors

$$\begin{aligned} f_1 &= (1,\ 1,\ 1,\ -1,\ 1,\ -1,\ -1,\ -1), \\ f_2 &= (1,\ -1,\ -1,\ -1,\ -1,\ -1,\ -1,\ 1), \end{aligned} \tag{B4}$$

with Fourier transforms

$$\begin{aligned} \hat{f}_1 &= \frac{1}{2}(0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 0,\ -1) \; , \\ \hat{f}_2 &= \frac{1}{2}(-1,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 0) \end{aligned} \tag{B5}$$

and Bell operators

$$\begin{aligned} B_{f_1} &= \frac{1}{2}\big(A_1(0)A_2(0)A_3(1) + A_1(0)A_2(1)A_3(0) \\ &\quad +A_1(1)A_2(0)A_3(0) - A_1(1)A_2(1)A_3(1)\big) \; , \\ B_{f_2} &= \frac{1}{2}\big(- A_1(0)A_2(0)A_3(0) + A_1(0)A_2(1)A_3(1) \\ &\quad +A_1(1)A_2(0)A_3(1) + A_1(1)A_2(1)A_3(0)\big) \; . \end{aligned}$$

Luckily(?), for $n = 3$ half of the coordinates of vectors $\hat{f}$ in (B5) vanish. Thus, half of the experimental setups are not involved in the optimal operators B_f. Same situation happens for $n = 5$ particles.

Last example is for $n = 4$ with collection of even vectors $\mathcal{P}_4 = \{1100, 1010, 1001, 0110, 0101, 0011, 1111\}$ that produces the orbits

$$\begin{cases} f(0000) = -f(0011) = -f(0101) = -f(0110) \\ = -f(1001) = -f(1010) = -f(1100) = f(1111) \end{cases}$$

and

$$\begin{cases} f(0001) = f(0010) = f(0100) = -f(0111) \\ = f(1000) = -f(1011) = -f(1101) = -f(1110) \end{cases}$$

The choice of sign $f(0000) = f(0001) = 1$ in the orbits gives the optimal vector

$$f = (1, 1, 1, -1, 1, -1, -1, -1, 1, -1, -1, -1, -1, -1, -1, 1)$$

with Fourier transform

$$\hat{f} = \frac{1}{4}(1, -1, -1, -1, -1, -1, -1, 1, -1, -1, -1, 1, -1, 1, 1, 1) \tag{B6}$$

and a Bell operator with sixteen products of four observables each. The reader may construct B_f himself by using (3) with the optimal vector (B6).

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